

Technical Appendix F

Additional Information on Flag Fields

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1. Introduction

A comprehensive check has been performed on the various flag fields in the Risk- Screening Environmental Indicators model, to ensure that the fields are correct and that any change in the status of any chemicals has been properly accounted for. Effective October of 1999, the fields in the model are in accordance with the sources listed below. The fields in the model which were checked are as follows:

- 33/50 Flag
- HAP Flag
- CAA Flag
- CERCLA Flag
- Priority Pollutant Flag
- SDWA Flag
- OSHA Carcinogen
- (Year) Added
- Expansion
- Core
- Metal

The details of each check performed, the sources used, and any changes made to the RSEI model are given below.

2. 33/50 Flag

A list of the 17 chemicals targeted by EPA's 33/50 program was downloaded from <http://www.epa.gov/opptintr/tri/>. The document is entitled "1994 Toxics Release Inventory Public Data Release Box E-6: 17 Priority Chemicals Targeted by the 33/50 Program." No inconsistencies were found with the current (July 6 public) version of the model. Note that EPA's list contains 17 chemicals, but several of them correspond to multiple TRI chemicals. The following table lists certain chemicals and chemical categories as reported in EPA's 33/50 Program list, and the corresponding entries in the RSEI model, which were given 33/50 flags. Therefore, the RSEI model contains 24 chemicals with 33/50 flags.

Table F-1
Chemicals Regulated under the 33/50 Program with Multiple TRI Entries

Name in EPA's 33/50 List	Corresponding TRI Chemicals	CAS Numbers
Cadmium and compounds	Cadmium	7440-43-9
	Cadmium compounds	N078
Chromium and compounds	Chromium	7440-47-3
	Chromium compounds	N090
Cyanide compounds	Cyanide compounds	N106
	Hydrogen cyanide	74-90-8
Nickel and compounds	Nickel	7440-02-0
	Nickel compounds	N495
Xylenes	Xylenes (mixed isomers)	1330-20-7
	p-Xylene	106-42-3
	m-Xylene	108-38-3
	o-Xylene	95-47-6

3. HAP Flag

The list of original hazardous air pollutants (HAPs) was downloaded from <http://www.epa.gov/ttn/uatw/orig189.html>. The document is entitled “Unified Air Toxics Website- CAA: Original List of Hazardous Air Pollutants.”

A short list of changes to the HAP list was downloaded from <http://www.epa.gov/ttn/uatw/atwsmod.html>, and is entitled “Unified Air Toxics Website–CAA: Modifications to the 112(b) Hazardous Air Pollutants.” Both the original and modified lists were found on the Office of Air Quality Planning & Standards’ (OAQPS) Unified Air Toxics Website. The chemicals being modified (caprolactum and hydrogen sulfide) are not in the Environmental Indicators model. A third chemical, glycol ethers (CAS N230) is in the model; however, the

change (a change in definition) is being proposed and is not final at this time (its listing as a HAP has not changed). Table F-2 presents the changes made to the HAP flag field.

Table F-2
Changes to ‘HAP’ Flag Field

CAS Number	Chemical	Change Made
79-06-1	Acrylamide	Added HAP flag to model
67-66-3	Chlorform	Added HAP flag to model
58-89-9	Lindane	Added HAP flag to model
101-68-8	Methylenebis(phenylisocyanate) (MDI)*	Added HAP flag to model. Changed ‘Chemical’ field from blank to ‘4,4’-Diphenylmethane diisocyanate’
7803-51-2	Phosphine	Added HAP flag to model
7723-14-0	Phosphorus	Added HAP flag to model
123-38-6	Propionaldehyde	Added HAP flag to model
100-44-7	Benzyl Chloride	Added HAP flag to model
98-88-4	Benzoyl Chloride	Removed HAP flag from model

* Note that in 1995 MDI’s status was changed from that of a single chemical to a member of the Diisocyanates (N120). However, it is still included in the RSEI model as a single chemical for historical reasons, so that releases in previous years can be examined.

4. CAA Flag and CERCLA Flag

A list of the chemicals regulated under the Clean Air Act (CAA) and the Comprehensive Environmental Response, Compensation, and Liability Act of 1980/Superfund (CERCLA) was downloaded from <http://www.epa.gov/ceppo/pubs/title3.pdf>. The title of the document is “Title III List of Lists (EPA 550-B-98-017, November 1998).” The list of CAA- and CERCLA-regulated chemicals is located on pages 1 through 36 of this document. Table F-3 presents the changes made to these two flag fields.

Table F-3
Changes to ‘CAA’ and ‘CERCLA’ Flag Fields

CAS Number	Chemical	Change Made
75-07-0	Acetaldehyde	Added CAA flag to model Added CERCLA flag to model
101-68-8	Methylenebis(phenylisocyanate) (MDI)*	Added CERCLA flag to model
105-67-9	2,4 Dimethylphenol	Added CERCLA flag to model
10049-04-4	Chlorine dioxide	Added CAA flag to model
23564-08-5	Thiophanate-methyl	Added CERCLA flag to model.
128-03-0	Potassium dimethyldithiocarbamate	Removed CERCLA flag from model
128-04-1	Sodium dimethyldithiocarbamate	Removed CERCLA flag from model
137-41-7	Potassium N-methyldithiocarbamate	Removed CERCLA flag from model
137-42-8	Metham Sodium	Removed CERCLA flag from model
533-74-4	Dazomet	Removed CERCLA flag from model
759-94-4	Ethyl dipropylthiocarbamate (EPTC)	Removed CERCLA flag from model
1114-71-2	Butylethylcarbamothioic acid S-propyl ester (Pebulate)	Removed CERCLA flag from model
1134-23-2	Cycloate	Removed CERCLA flag from model
2212-67-1	1H-Azepine-1 carbothioic acid, hexahydro-S-ethyl ester (Molinate)	Removed CERCLA flag from model
7647-01-0	Hydrochloric acid	Removed CAA flag from model
14484-64-1	Tris(dimethylcarbamodithioato-S,S')iron (Ferbam)	Removed CERCLA flag from model
55406-53-6	3-Iodo-2-propynyl butylcarbamate	Removed CERCLA flag from model

* Note that in 1995 MDI's status was changed from that of a single chemical to a member of the Diisocyanates (N120). However, it is still included in the RSEI model as a single chemical for historical reasons, so that releases in previous years can be examined.

Several chemicals have multiple entries in the Title III List of Lists. In most cases, the different entries for one chemical (as identified by the CAS number) are classified the same regarding CAA and CERCLA. However, for a few chemicals, the various forms of the chemical are regulated differently. In one case, that of hydrochloric acid (see above), this resulted in a change in the model for the CAA flag field. The details for hydrochloric acid and other chemicals, which did not result in changes to this field, are given below in Table F-4.

Table F-4
Chemicals with Multiple Entries in List of Lists

CAS Number	Chemical	Description in Form R	Description of form(s) in List of Lists
7647-01-0	Hydrochloric acid	acid aerosols, including mists, vapors, gas, fog, and other airborne particles of any size.	Form chosen: Hydrochloric acid (aerosol forms only) - regulated only under CERCLA. Other forms regulated differently are Hydrochloric acid (conc. 37% or greater); Hydrogen chloride (anhydrous); and Hydrogen chloride (gas only), which are also regulated under the CAA.
7664-41-7	Ammonia	includes anhydrous ammonia and aqueous ammonia from water dissociable ammonium salts and other sources; 10 percent of total aqueous ammonia is reported under this listing.	Form chosen: Ammonia (anhydrous) - regulated under both CERCLA and CAA. Ammonia is regulated under CERCLA only; Ammonia (conc. 20 % or greater) is regulated under both CERCLA and CAA.
7664-39-3	Hydrogen fluoride	No description	Form chosen: Hydrogen fluoride - regulated under CERCLA only. Only other form is Hydrogen fluoride (anhydrous)-regulated under both CAA and CERCLA.
7697-37-2	Nitric acid	No description	Form chosen: Nitric acid - regulated under CERCLA only. Only other form is Nitric acid (conc 80% or greater)-regulated under both CERCLA and CAA.

5. Priority Pollutant Flag

The list of priority toxic pollutants was downloaded from <http://www.epa.gov/ost/pc/revcom.pdf>. This file is entitled “National Recommended Water Quality Criteria” and is a publication of U.S. EPA Office of Water (EPA 822-Z-99-001, April 1999). The list of priority pollutants is found on pages 7 through 13. Table F-5 presents the changes made to this flag field.

Table F-5
Changes to ‘Priority Pollutant’ Flag Field

CAS Number	Chemical	Change Made
105-67-9	2,4-Dimethylphenol	Added Priority Pollutant flag to model.
319-84-6	alpha-Hexachlorocyclohexane	Added Priority Pollutant flag to model.
542-75-6	1,3-Dichloropropylene	Added Priority Pollutant flag to model.
71-55-6	1,1,1-Trichloroethane	Added Priority Pollutant flag to model.
74-87-3	Chloromethane	Added Priority Pollutant flag to model.
75-34-3	Ethylidene dichloride	Added Priority Pollutant flag to model.
75-35-4	Vinylidene chloride	Added Priority Pollutant flag to model.
79-00-5	1,1,2-Trichloroethane	Added Priority Pollutant flag to model.
87-68-3	Hexachloro-1,3-butadiene	Added Priority Pollutant flag to model.
N090*	Chromium compounds	Added Priority Pollutant flag to model.

*EPA’s Priority Pollutant list includes Chromium III (CAS# 16065-83-1) and Chromium VI (CAS# 18540-29-9). The TRI inventory does not report Chromium in the same way: only Chromium (CAS# 7440-47-3) and Chromium compounds are reported. Both of these chemicals have been flagged in the RSEI model as priority pollutants.

6. SDWA Flag

The list of chemicals regulated under the Safe Drinking Water Act (SDWA) was downloaded from <http://www.epa.gov/OGWDW/wot/appa.html>. The document is entitled “National Primary Drinking Water Regulations” and lists chemicals regulated under either national primary or national secondary drinking water standards. The SDWA flag in the model is indicative of either primary or secondary standards. Table F-6 presents the changes that have been made to this flag field.

Table F-6
Changes to ‘SDWA’ Flag Field

CAS Number	Chemical	Change Made
7429-90-5	Aluminum (fume or dust)	Added SDWA flag to model (represents secondary standard only).*
7440-22-4	Silver	Added SDWA flag to model (represents secondary standard only).*
2164-07-0	Dipotassium endothall	Added SDWA flag to model.**
116-06-3	Aldicarb	Removed SDWA flag from model.
7440-02-0	Nickel	Removed SDWA flag from model.

* These changes make these chemicals consistent with the previous treatment of zinc, which was marked as an SDWA chemical for a secondary standard only.

** EPA lists ‘Endothall,’ which is not a TRI chemical. However, Dipotassium endothall is reported in TRI; being a salt of Endothall, it was flagged as an SDWA pollutant.

Note that three of the four chemicals in the Total Trihalomethanes category in the SDWA list are TRI chemicals, and therefore are flagged in the model as SDWA chemicals. These chemicals are Chloroform (CAS# 67-66-3), Bromoform (CAS# 75-25-2), and Dichlorobromomethane (CAS# 75-27-4). Dibromochloromethane (CAS# 124-48-1) is not a TRI chemical.

7. OSHA Carcinogen Flag

The list of OSHA carcinogens was downloaded from <http://www.epa.gov/opptintr/tri/oshacarc.pdf>, a pdf file entitled “Box 2-4. Basis of OSHA Carcinogen Listing for Individual Chemicals.” The year of the publication from which this is taken was not provided, but this listing is reflected in the 1997 TRI Public Data Release. This table is located on pages 41 and 42. Table F-7 presents the changes that were made to the OSHA Carcinogen flag field.

Table F-7
Changes to ‘OSHA Carcinogen’ Flag Field

CAS Number	Chemical	Change Made
121-14-2	Dinitrotoluene	Removed OSHA Carcinogens flag from model.
606-20-2	2,6-Dinitrotoluene	Removed OSHA Carcinogens flag from model.
98-95-3	Nitrobenzene	Removed OSHA Carcinogens flag from model.

8. Year Added

Please note that ‘core’ refers to chemicals that were added in 1987 AND have had no changes in reporting requirements since that time (although the base year for the RSEI’ model is 1988). ‘Expansion’ refers to chemicals that were added for reporting year 1995; the term does not refer to chemicals added in other years. The ‘Year Added’ field was checked against the 1998 Code of Federal Regulations (40CFR372)¹. The changes made are summarized in Table F-8.

¹ There are two tables in the CFR that list the chemicals reported under TRI- one table organized alphabetically by chemical, the other numerically by CAS number. Note that while they are supposed to contain the identical chemicals, each list is missing two chemicals contained in the other list. The first, alphabetical list is missing Flumetralin (CAS 62924-70-3) and Ammonium sulfate (solution) (CAS 7783-20-2). The second list is missing Toluene-2,4-diisocyanate (CAS 584-84-9) and Vinyl bromide (CAS 593-60-2). It is assumed that the complete list includes all four of these chemicals. Therefore, there are 583 chemicals and 28 chemical categories listed in the CFR.

Table F-8
Changes to (Year) ‘Added’ Field

CAS Number	Chemical	Change Made
101-68-8	Methylenebis(phenylisocyanate) (MDI)	‘Added’ field changed from 1995 to 1987.*
306-83-2	2,2-Dichloro-1,1,1-trifluoroethane	‘Added’ field changed from 1987 to 1994.
354-23-4	1,2-Dichloro-1,1,2-trifluoroethane	‘Added’ field changed from 1987 to 1994.
354-25-6	1-Chloro-1,1,2,2-tetrafluoroethane	‘Added’ field changed from 1987 to 1994.
812-04-4	1,1-Dichloro-1,2,2-trifluoroethane (HCFC-123b)	‘Added’ field changed from 1987 to 1994.
2837-89-0	2-Chloro-1,1,1,2-tetrafluoroethane	‘Added’ field changed from 1987 to 1994.
90454-18-5	Dichloro-1,1,2-trifluoroethane	‘Added’ field changed from 1987 to 1994.

* Note that in 1995 MDI’s status was changed from that of a single chemical to a member of the Diisocyanates (N120). However, it is still included in the RSEI model as a single chemical for historical reasons, so that releases in previous years can be examined.

While most chemicals in the CFR have an effective date of January in a given year, several chemicals became effective in July. In these cases, the ‘Added’ field in the RSEI model contains the following year.

Four chemicals which were listed in the CFR were not found in the model. They are shown in Table F-9.

Table F-9
Chemicals in the 1998 CFR but Not in the RSEI Model

CAS Number	Chemical	Note
74-93-1	Methyl mercaptan	Chemical was delisted.
10222-01-2	2,2-Dibromo-3-nitrilopropionamide	Under administrative stay.
7783-06-4	Hydrogen sulfide	Chemical was delisted.
62924-70-3	Flumetralin	

9. Expansion Flag

To confirm the Expansion flag, that field was checked against the November 30, 1994 Federal Register notice adding chemicals to the TRI reporting program.

All of the chemicals marked with a flag in the RSEI model were listed as being added in 1995 in the Federal Register notice. However, the following chemicals from the Federal Register notice were not found in the model.

Table F-10
Chemicals in Expansion FR Notice Not Found in Model

CAS Number	Chemical	Note
52-51-7	Bronopol	Chemical was delisted.
10222-01-2	2,2-Dibromo-3-nitrilopropionamide	Chemical is under administrative stay.
75-78-5	Dimethyldichlorosilane	Chemical has been voluntarily remanded from the TRI reporting list.
576-26-1	2,6-Dimethylphenol	Chemical was delisted.
75-79-6	Methyltrichlorosilane	Chemical has been voluntarily remanded from the TRI reporting list.
75-77-4	Trimethylchlorosilane	Chemical has been voluntarily remanded from the TRI reporting list.

10. Core Chemical Flag

To confirm that all flags marked as ‘Core’ are correct, all chemicals with 1987 as the year added (confirmed under (Year) Added flag) without being marked as ‘Core’ were checked. Seven chemicals shown in Table F-11 were found. All were mentioned in a 1996 memorandum entitled ‘TRI Environmental Indicators: Resolution of Certain TRI Reporting Issues with TRIB Staff’ as having had changes in their reporting requirements; thus, they are correct in not being marked as ‘Core.’

In addition, all chemicals marked as ‘Core’ in the model were compared against Table 3-8A in the 1997 Toxics Release Inventory Public Data Release (PDR). Any chemicals marked as having changes in reporting requirements were not considered to be ‘Core.’ No discrepancies were found; however, 42 chemicals in the model were not found in the table in the 1997 PDR because they did not have any 1997 releases (according to the model). Ten of these 42 chemicals did have releases in years other than 1997, and so these were checked against the 1987-1996 TRI Release Inventory CD, and found to be marked ‘Core.’

Table F-11
Chemicals in RSEI Model Added in 1987 but Not Marked as ‘Core’

CAS Number	Chemical
101-68-8	Methylene bis(phenylisocyanate) (MDI)
1344-28-1	Aluminum oxide (fibrous forms)
6484-52-2	Ammonium nitrate (solution)
7647-01-0	Hydrochloric acid (aerosol)
7664-41-7	Ammonia
7664-93-9	Sulfuric acid (aerosol)
7783-20-2	Ammonium sulfate

Note that while Glycol ethers (CAS N230) had a clarification of definition effective in 1995, it was originally added in 1987 and is still considered a core chemical by the model and the TRI Public Data Release.

11. Metal Flag

Finally, the ‘Metal’ field was checked against the ‘Core’ field (already confirmed above) as well as against an internal file of compounds considered metals. No changes were needed to the ‘Metal’ field.

12. Summary of Data Sources

The following table provides information on the sources of data used to identify the various flags in the model.

Table F-12
Summary of Data Sources

Flag	Access Address	Date Accessed	Title
33/50	http://www.epa.gov/opptintr/tri/	9/29/99	1994 Toxics Release Inventory Public Data Release Box E-6. 17 Priority Chemicals Targeted by the 33/50 Program
HAP	http://www.epa.gov/ttn/uatw/orig189.html		Unified Air Toxics Website-CAA: Original List of Hazardous Air Pollutants
CAA	http://www.epa.gov/ceppo/pubs/title3.pdf		Title III List of Lists
Priority Pollutant	http://www.epa.gov/ost/p/c/revcom.pdf		National Recommended Water Quality Criteria
SDWA	http://www.epa.gov/OGWDW/wot/appa.html		National Primary Drinking Water Regulations
CERCLA	http://www.epa.gov/ceppo/pubs/title3.pdf		Title III List of Lists
OSHA	http://www.epa.gov/opptintr/tri/oshacarc.pdf		Box 2-4. Basis of OSHA Carcinogen Listing for Individual Chemicals
Year Added	Code of Federal Regulations, Part 40, Section 372.	10/12/99	
Expansion	Federal Register, November 30, 1994	10/12/99	
Core Chemical	Code of Federal Regulations, Part 40, Section 372. TRI Release Inventory, 1987-1996	10/12/99 10/18/99	
Metal	Internal file (TRI_TOME.wk4)	10/4/99	